

Validation of the STable AutoCorrelation Integral Estimator (STACIE) Using The AutoCorrelation Integral Drill (ACID) Test Set

model: exppoly(0, 2)

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1. Description of Figures and tables

The following sections contain figures and tables with the same type of results in each section, but computed for different kernels. All figures and tables are labeled with a letter and are explained below. For a full discussion of the results, we refer to the STACIE paper. [1]

(a) Illustration of input data.

- Left: an example input sequences (first 100 steps).
- Center: the sampling autocorrelation function (ACF) of the input data ($N = 1024$, $M = 256$, purple line) and the analytical ACF (dashed line).
- Right: the sampling power spectral density (PSD) of the input data ($N = 1024$, $M = 256$, turquoise line) and the analytical PSD (dashed line).

(b) Scaling of uncertainty of the autocorrelation integral with input data.

- The slope of the slanted gray lines indicates the ideal scaling of the uncertainty (proportional to $\frac{1}{\sqrt{NM}}$). The spacing between the lines corresponds to a factor of 2 in the uncertainty, the ideal case when changing N by a factor of 4.
- A square represents the standard deviations over 64 repetitions of STACIE's estimate of the autocorrelation integral for a specific combination of N and M .
- The dotted lines represent the corresponding predicted uncertainties.

(c) Assessment of the error estimate of the autocorrelation integral.

- The square blocks show the ratio of the standard deviation of the STACIE estimate and the RMS value of the predicted uncertainty, over 64 repetitions. This value is ideally 100%. Lower values mean that STACIE's predictions have a smaller spread than the predicted uncertainty.
- The dots show the ratio of the mean error and the RMS value of the predicted uncertainty, over 64 repetitions. This value is ideally 0%.

(d) Validation of the Maximum A Posteriori (MAP) estimate.

- The MAP estimate for the autocorrelation integral (blue, cross is the maximizer, ellipse is the 2-sigma volume).
- The Monte Carlo samples of the posterior distribution of the model parameters (black points).
- The mean and covariance of the Monte Carlo samples (red, cross is the mean, ellipse is the 2-sigma volume).

(e) Sensitivity of the autocorrelation integral to the cutoff frequency.

- This plot shows how the autocorrelation integral correlates with the effective number of points used in the fit (top) and the cutoff frequency (bottom).
- Results are shown only for the $M = 64$.
- The color code for different N corresponds to the legends shown in figures (b), (c), (d) and (e).

(f) Number of successful test cases (Failures are typically due to not finding any cutoff frequency with acceptable results.)

(g) Sanity check counts for the effective number of points

- Number of test cases for each combination of N and M where the effective number of points used in the fit is below $20P = 40$.

(h) Sanity check counts for the regression cost z-score

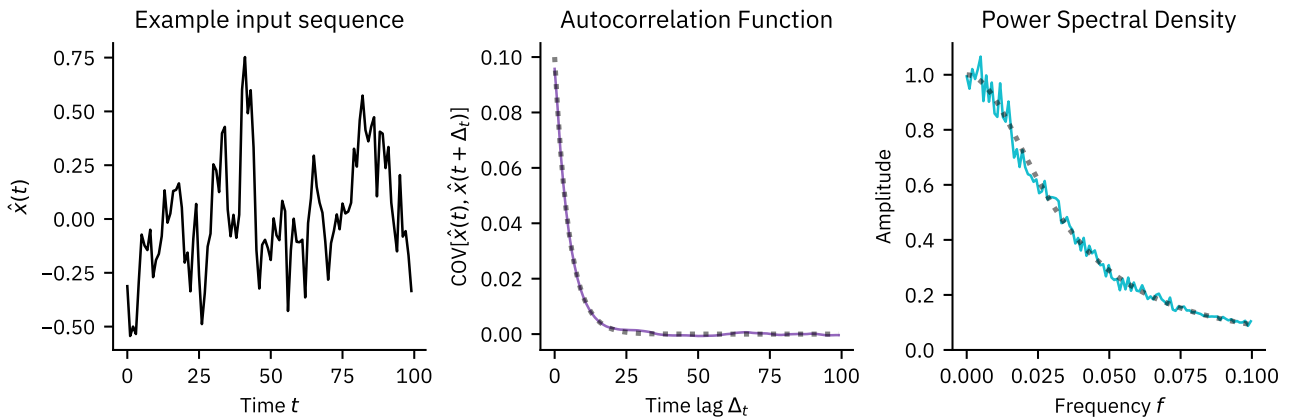
- Number of test cases for each combination of N and M where the z-score of the regression cost exceeds 2.

(i) Sanity check counts for the cutoff criterion z-score

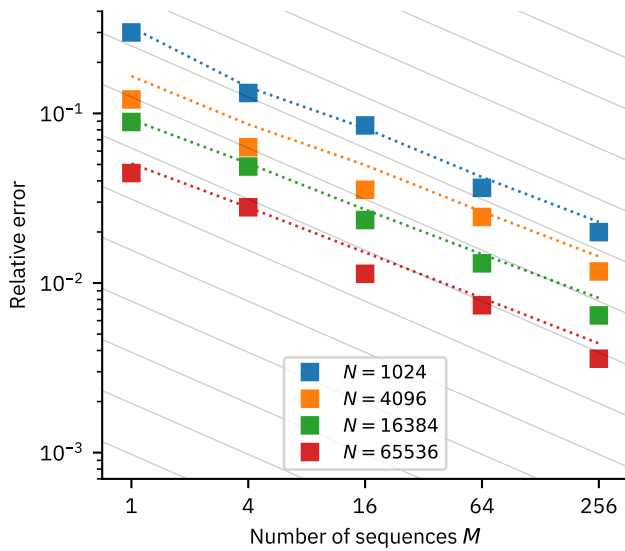
- Number of test cases for each combination of N and M where the z-score of the cutoff criterion exceeds 2.

2. Kernel exp1p

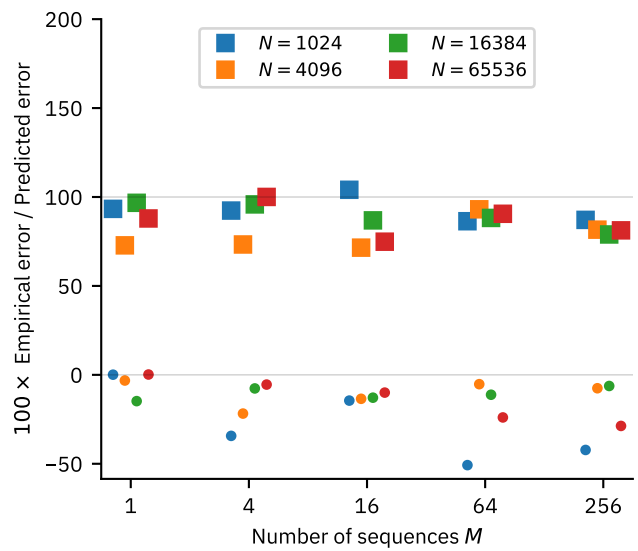
(a) Illustration of input data



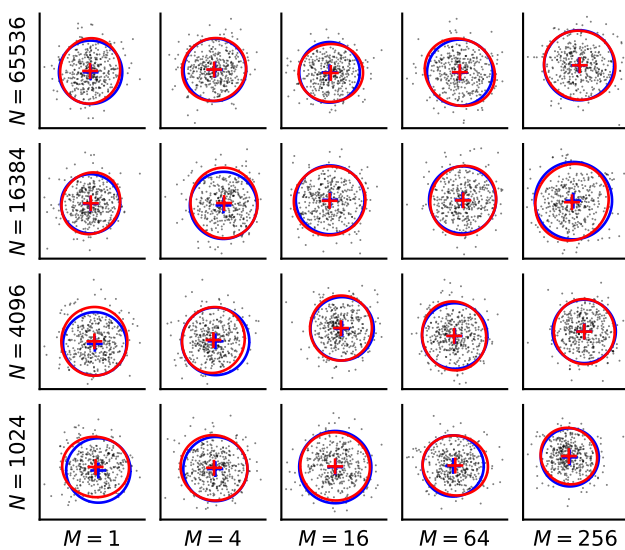
(b) Scaling of uncertainty of the autocorrelation integral with input data



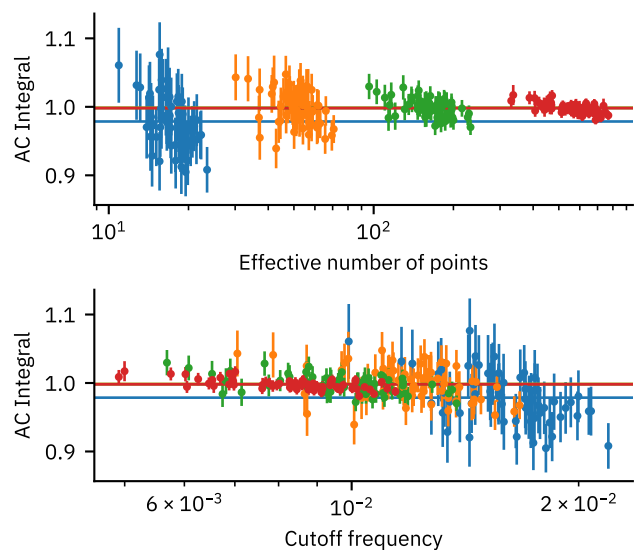
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	55	64	64	64	64
$N = 4096$	0	0	2	5	19
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

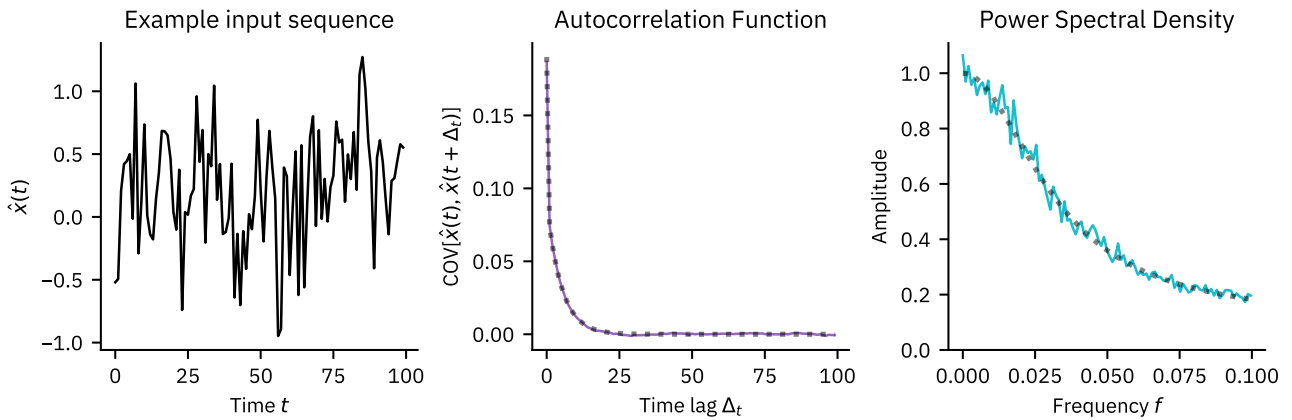
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	0	0	0	0
$N = 4096$	0	1	0	0	1
$N = 16384$	0	0	0	0	2
$N = 65536$	0	0	2	0	0

(i) Sanity check counts for the cutoff criterion z-score

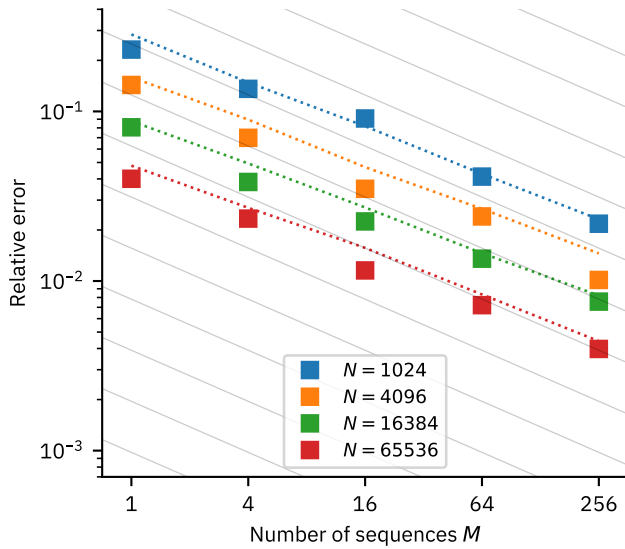
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	1	1	3	2	5
$N = 4096$	0	0	1	1	1
$N = 16384$	0	0	0	0	2
$N = 65536$	0	0	1	0	0

3. Kernel exp1w

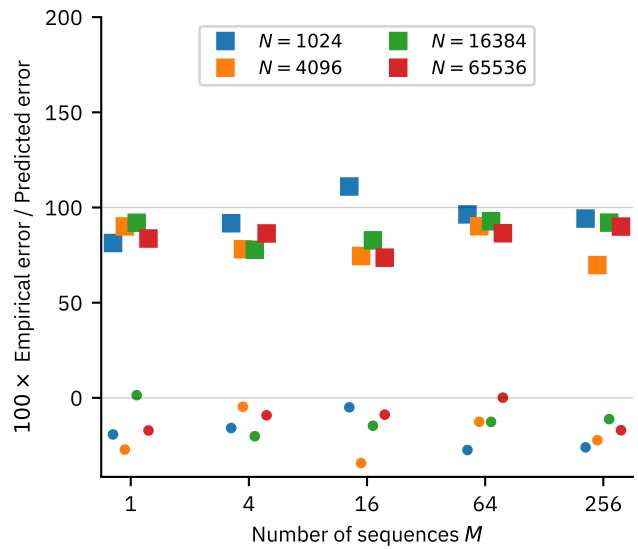
(a) Illustration of input data



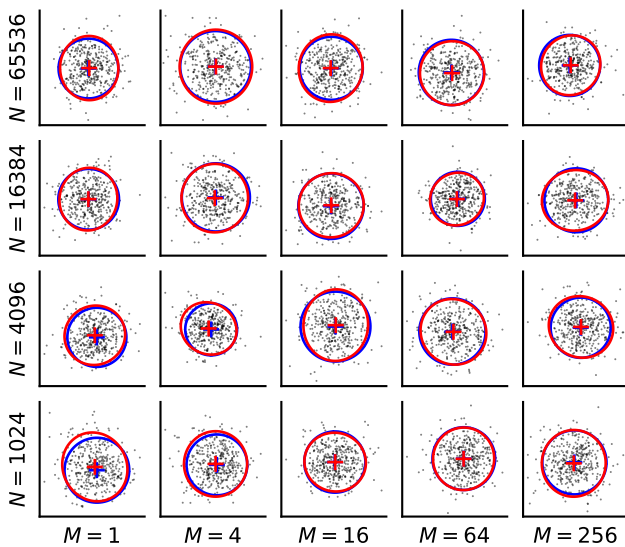
(b) Scaling of uncertainty of the autocorrelation integral with input data



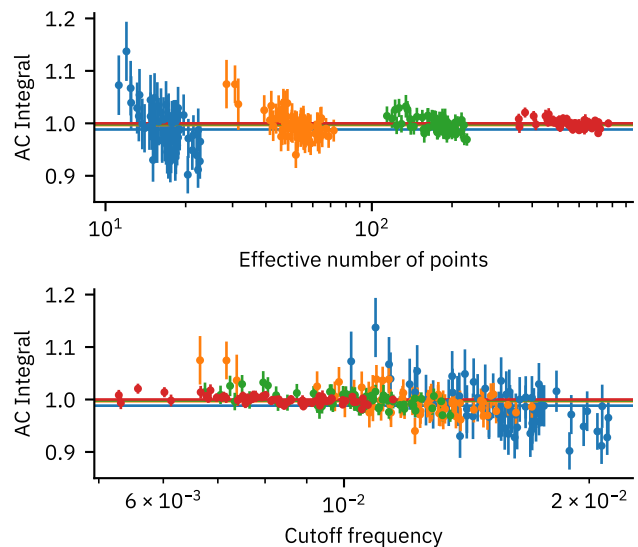
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	51	63	64	64	64
$N = 4096$	0	1	1	4	20
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

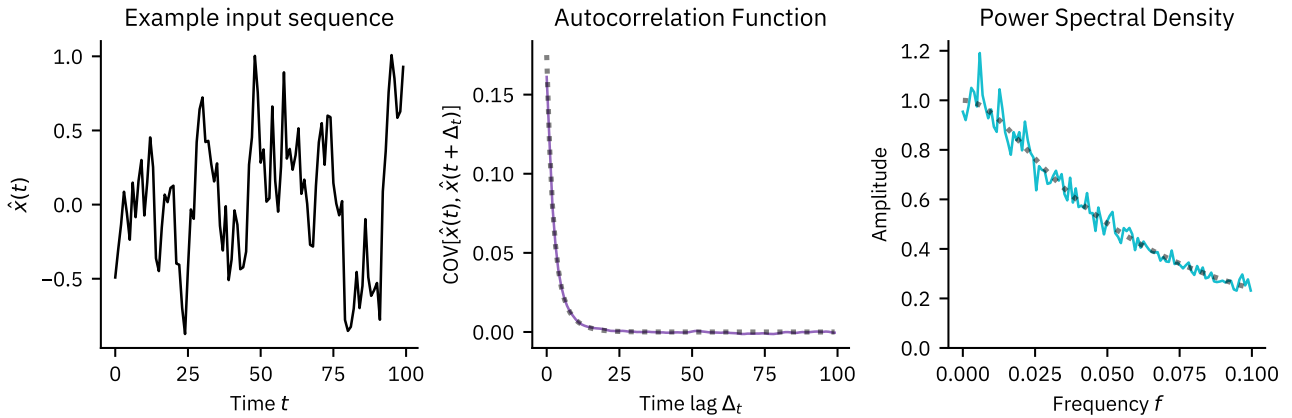
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	2	0	0	0
$N = 4096$	0	0	2	0	1
$N = 16384$	0	1	1	1	2
$N = 65536$	0	0	1	1	2

(i) Sanity check counts for the cutoff criterion z-score

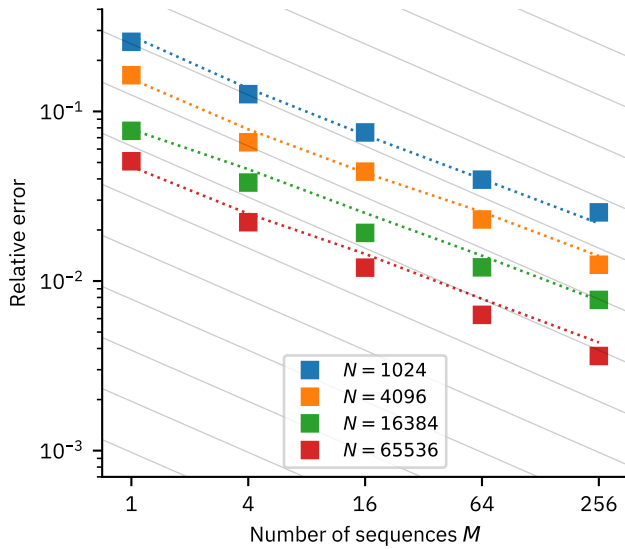
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	1	2	5	4	4
$N = 4096$	0	1	0	0	1
$N = 16384$	0	1	0	1	1
$N = 65536$	0	0	2	1	0

4. Kernel exp2

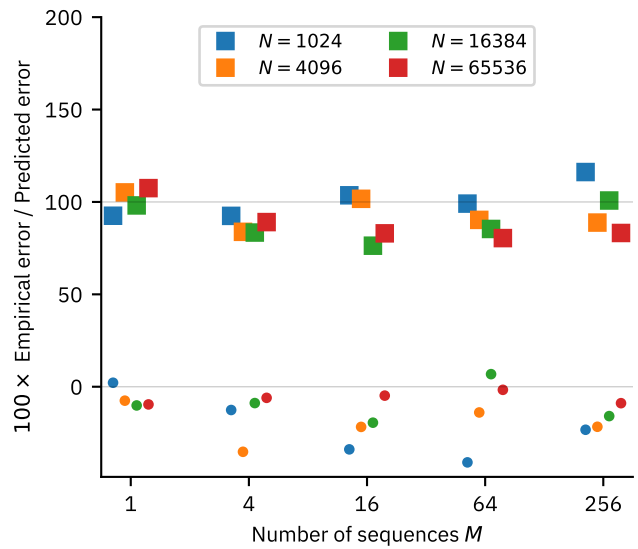
(a) Illustration of input data



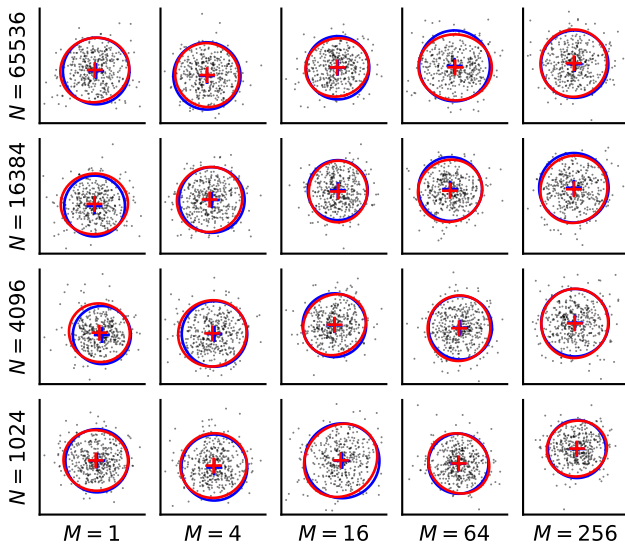
(b) Scaling of uncertainty of the autocorrelation integral with input data



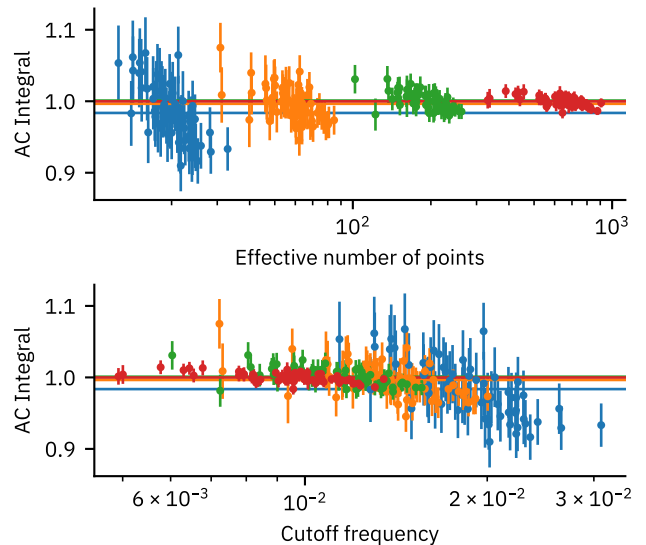
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	31	48	64	64	64
$N = 4096$	0	0	3	3	13
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

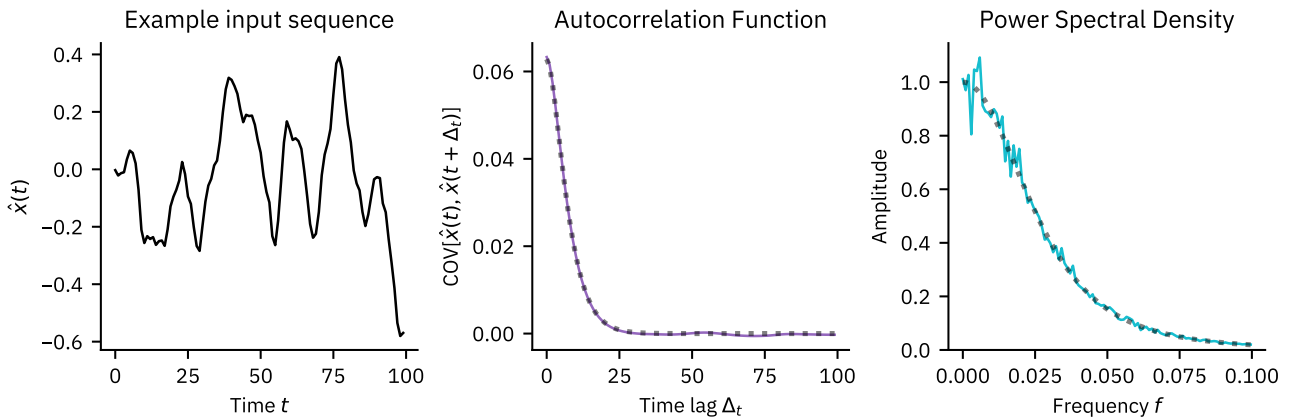
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	0	0	3	2
$N = 4096$	0	0	1	1	1
$N = 16384$	0	0	0	1	0
$N = 65536$	0	0	1	1	2

(i) Sanity check counts for the cutoff criterion z-score

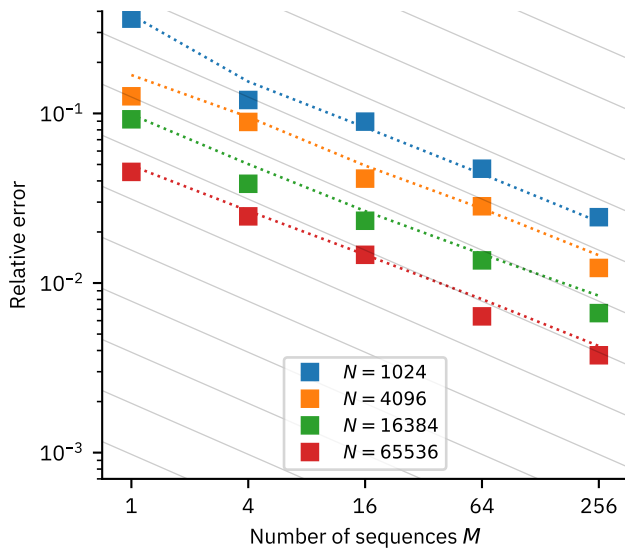
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	3	2	0	0	1
$N = 4096$	0	1	0	1	2
$N = 16384$	0	0	0	1	1
$N = 65536$	0	0	0	1	0

5. Kernel sho1pcrit

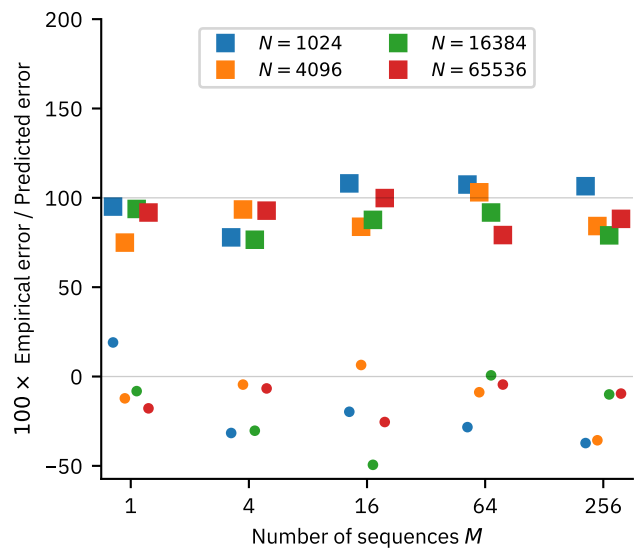
(a) Illustration of input data



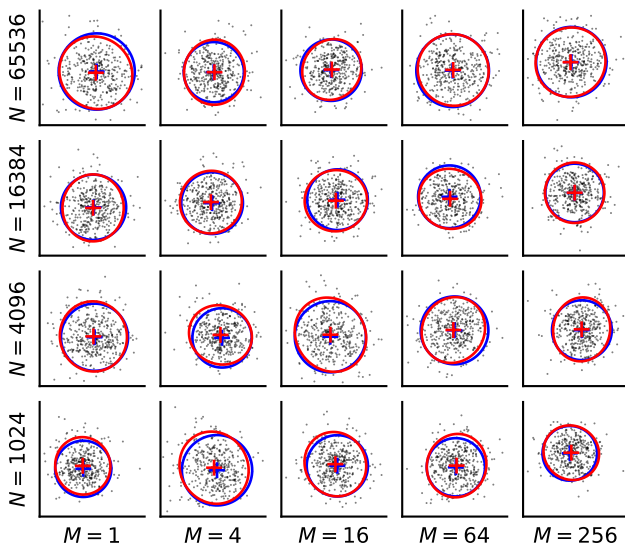
(b) Scaling of uncertainty of the autocorrelation integral with input data



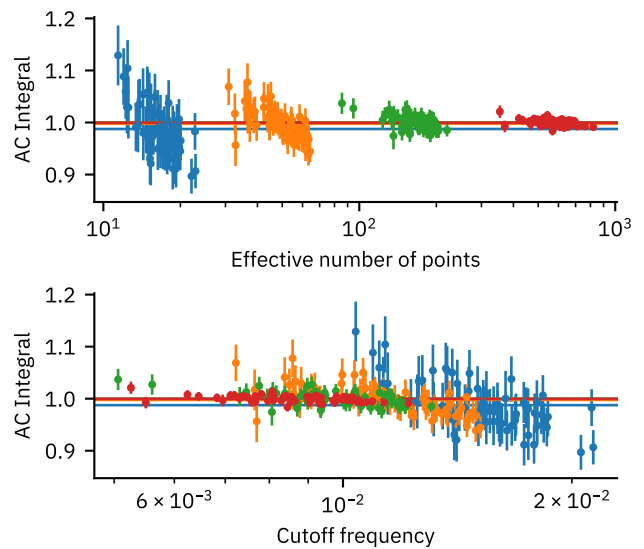
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	0	1	1	13	14
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

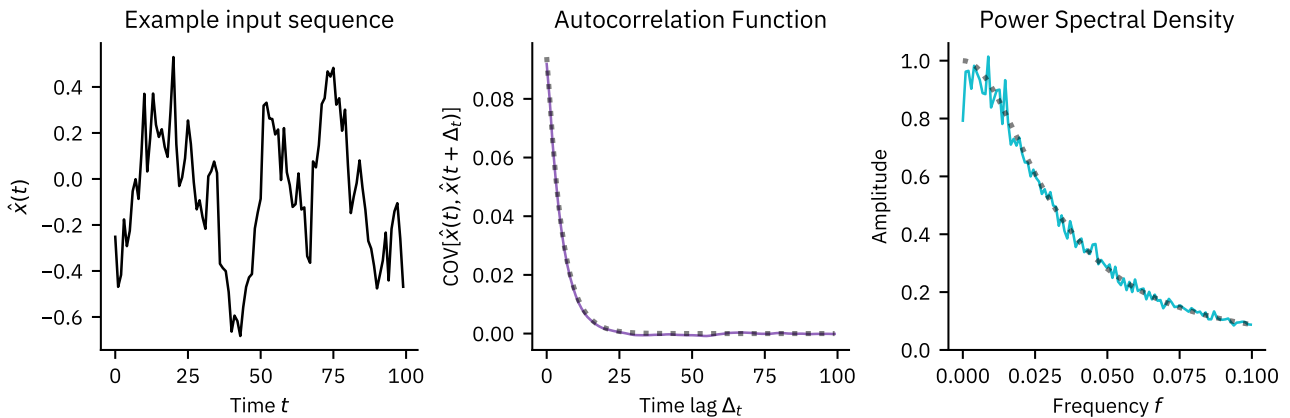
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	0	0	2	1
$N = 4096$	0	0	1	3	1
$N = 16384$	0	0	0	1	2
$N = 65536$	0	0	1	0	2

(i) Sanity check counts for the cutoff criterion z-score

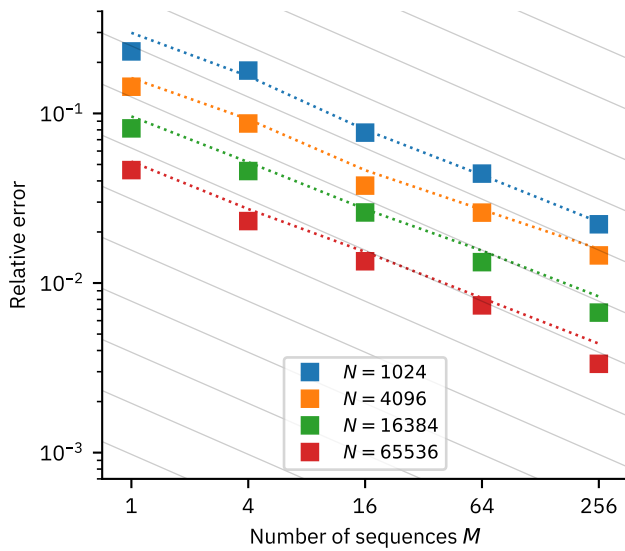
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	1	3	0	2	3
$N = 4096$	0	0	0	1	1
$N = 16384$	1	0	0	1	0
$N = 65536$	0	0	0	1	0

6. Kernel sho1pover

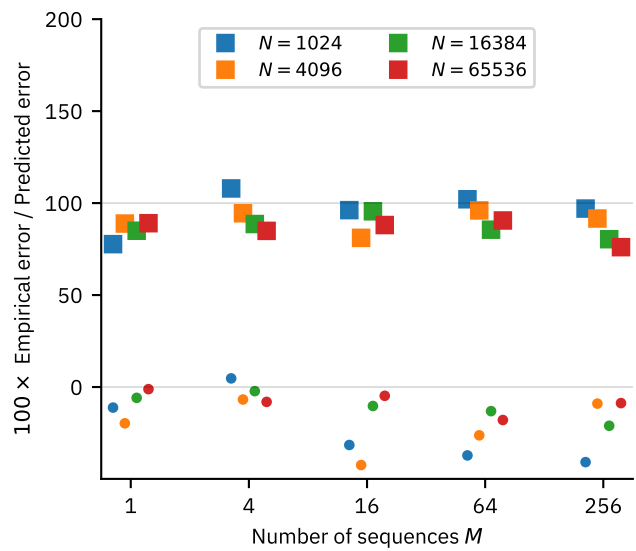
(a) Illustration of input data



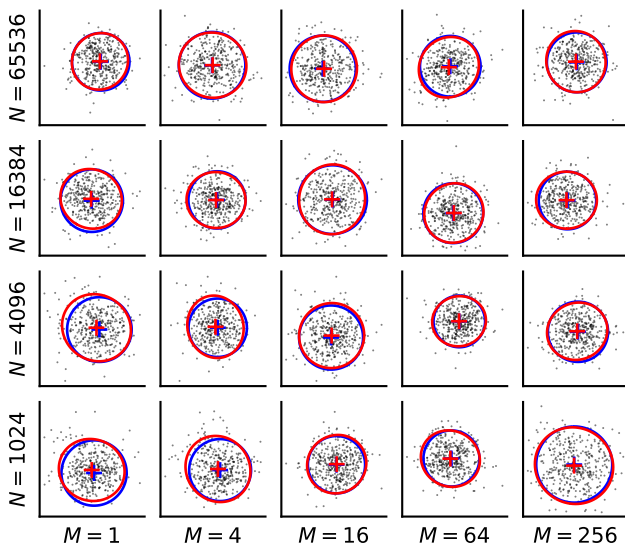
(b) Scaling of uncertainty of the autocorrelation integral with input data



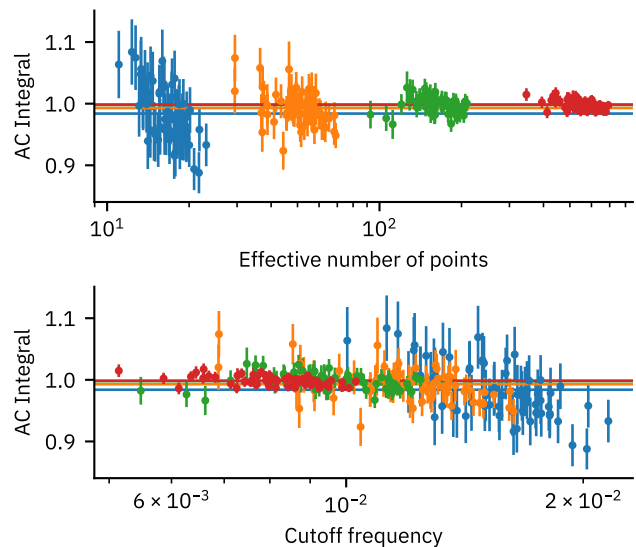
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	55	64	64	64	64
$N = 4096$	0	0	0	9	25
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

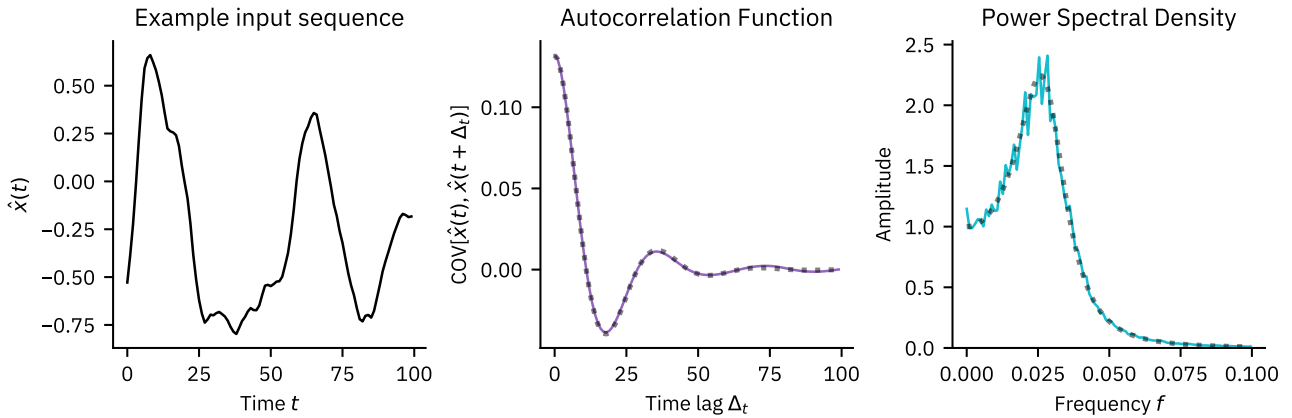
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	0	0	1	1
$N = 4096$	0	0	2	0	3
$N = 16384$	0	0	1	2	1
$N = 65536$	0	0	2	3	2

(i) Sanity check counts for the cutoff criterion z-score

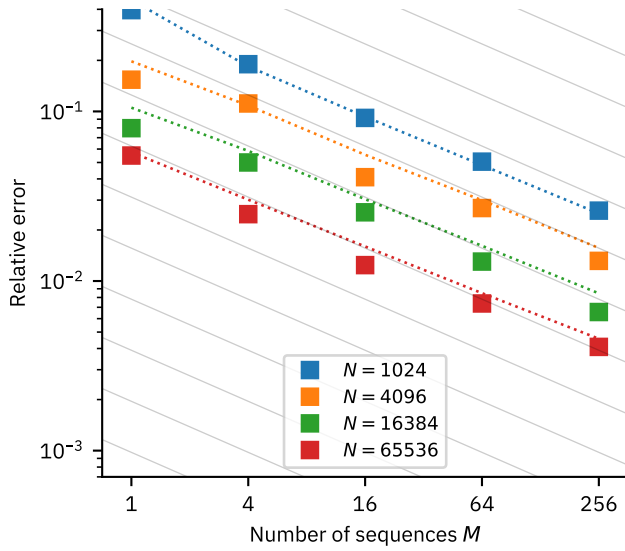
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	3	2	2	1	5
$N = 4096$	0	0	0	0	2
$N = 16384$	2	0	0	2	0
$N = 65536$	0	1	0	0	0

7. Kernel sho1punder

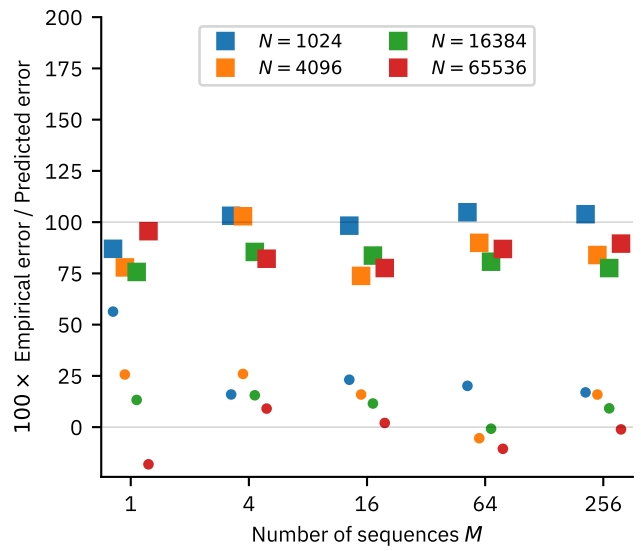
(a) Illustration of input data



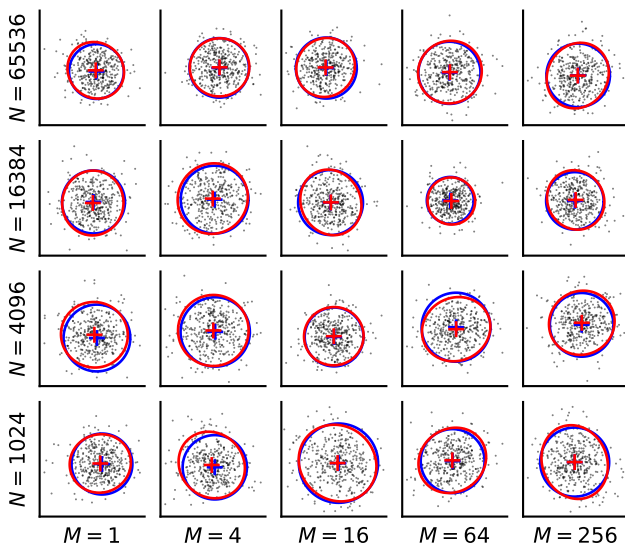
(b) Scaling of uncertainty of the autocorrelation integral with input data



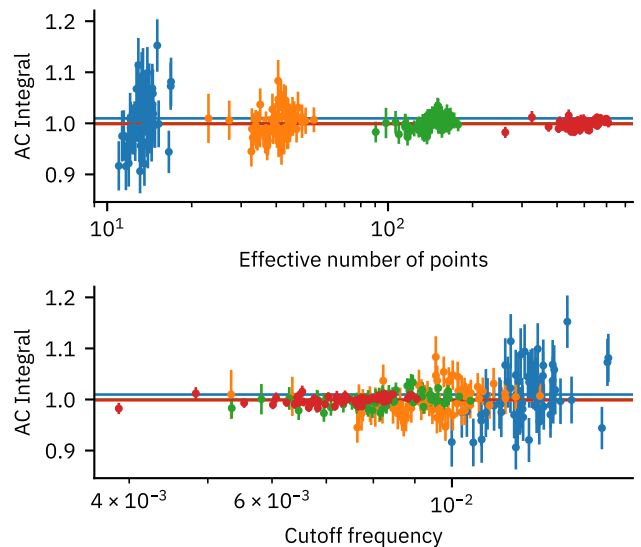
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	63	64	64	64	64
$N = 4096$	0	0	7	29	53
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

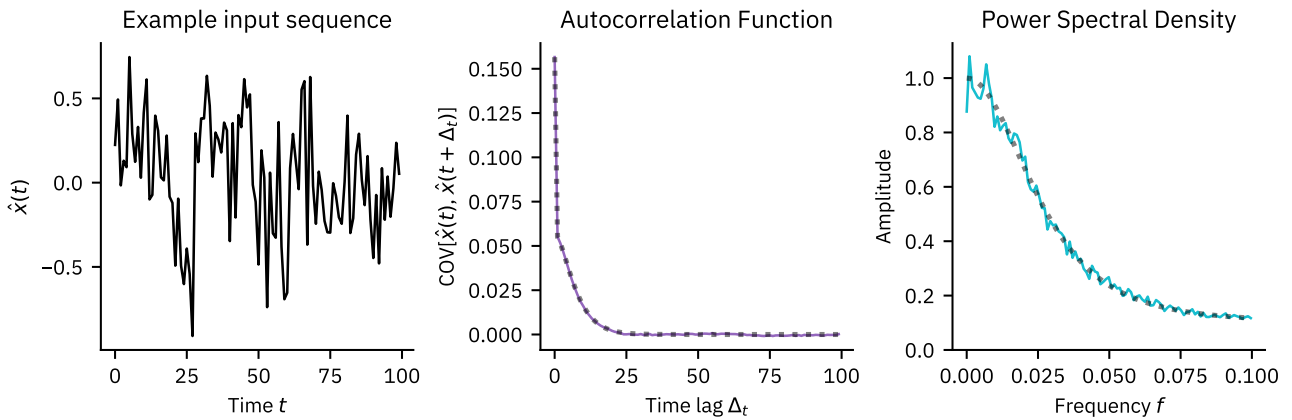
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	1	2	0	1
$N = 4096$	0	0	0	2	2
$N = 16384$	0	0	0	2	2
$N = 65536$	0	0	1	3	3

(i) Sanity check counts for the cutoff criterion z-score

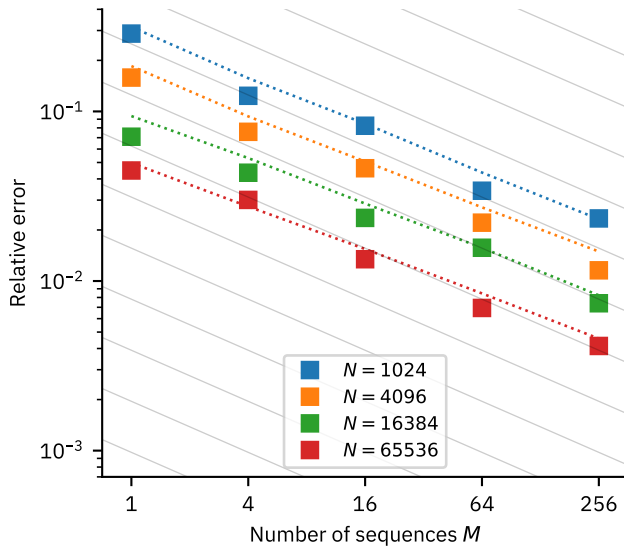
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	1	2	2	3	3
$N = 4096$	0	2	0	0	2
$N = 16384$	1	0	1	2	0
$N = 65536$	1	0	0	0	1

8. Kernel sho1wcrit

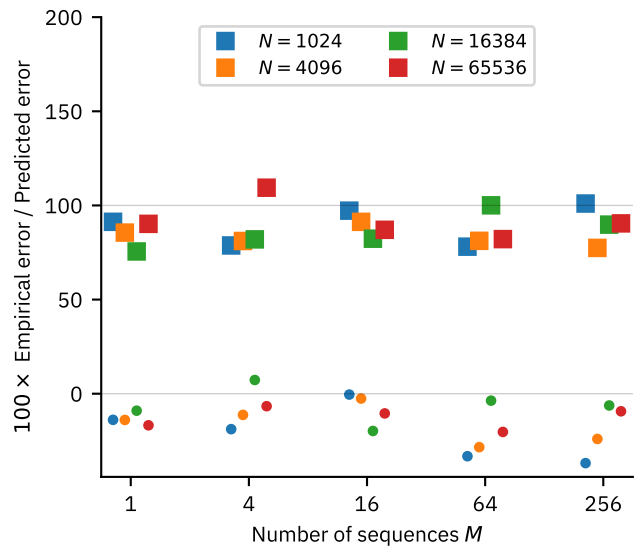
(a) Illustration of input data



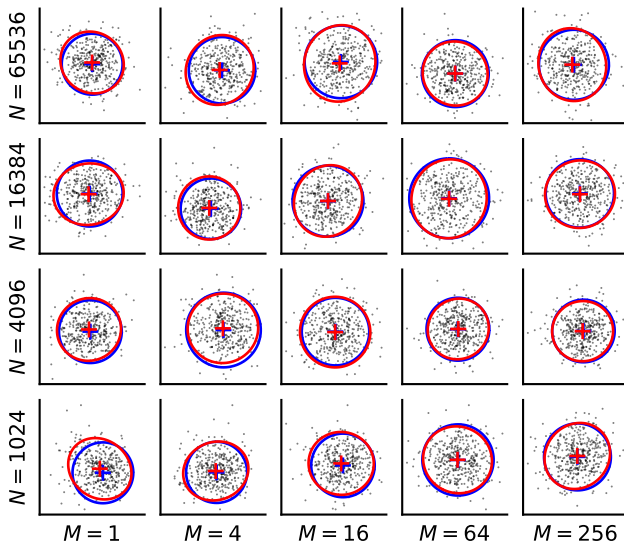
(b) Scaling of uncertainty of the autocorrelation integral with input data



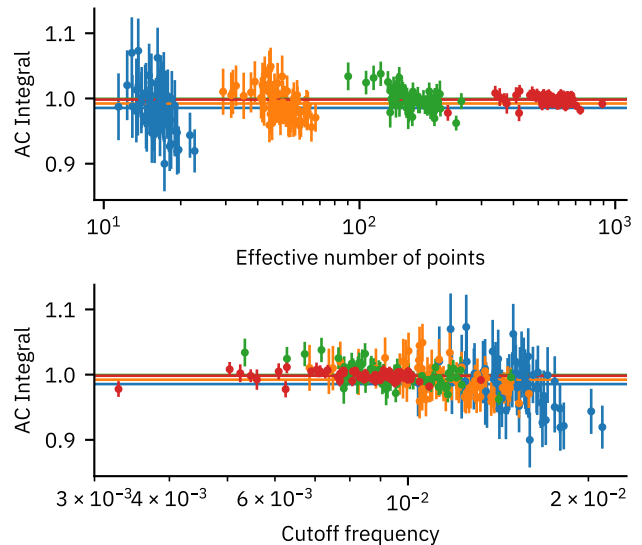
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	62	64	64	64	64
$N = 4096$	1	0	3	7	24
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

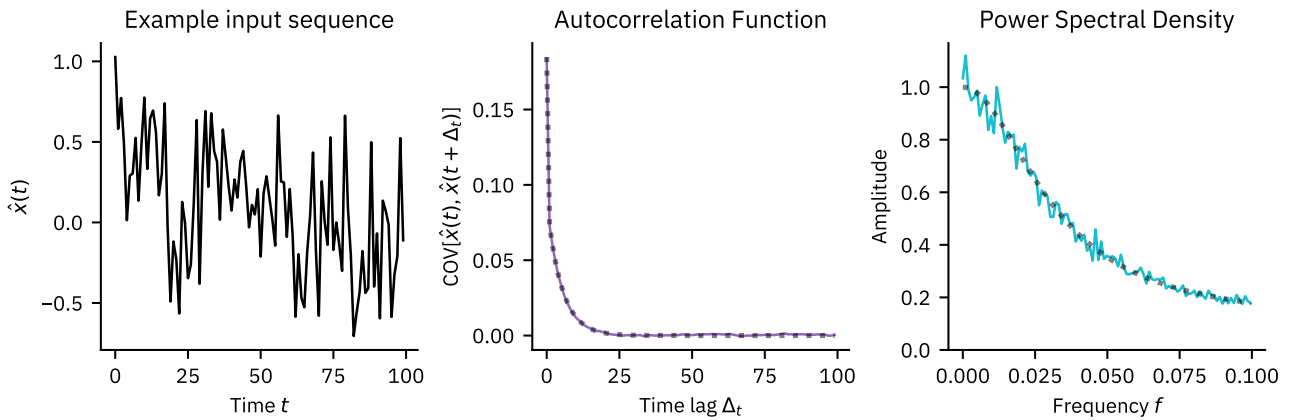
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	0	2	0	0
$N = 4096$	0	0	0	0	3
$N = 16384$	0	1	1	1	1
$N = 65536$	0	0	4	0	1

(i) Sanity check counts for the cutoff criterion z-score

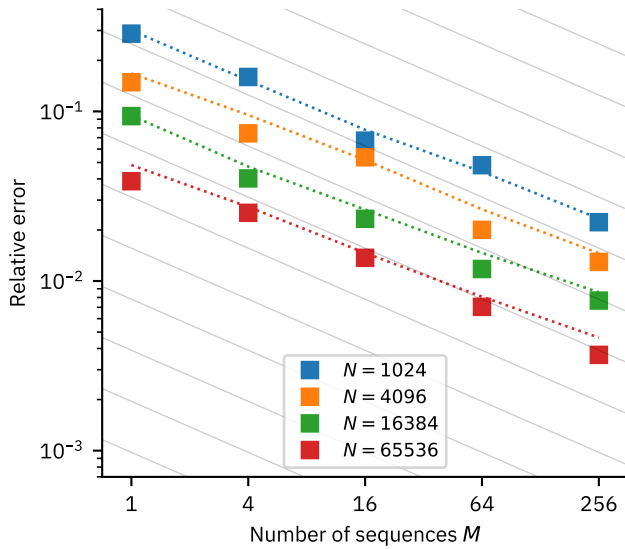
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	4	2	1	3	4
$N = 4096$	1	0	0	0	0
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	1	1	1

9. Kernel sho1wover

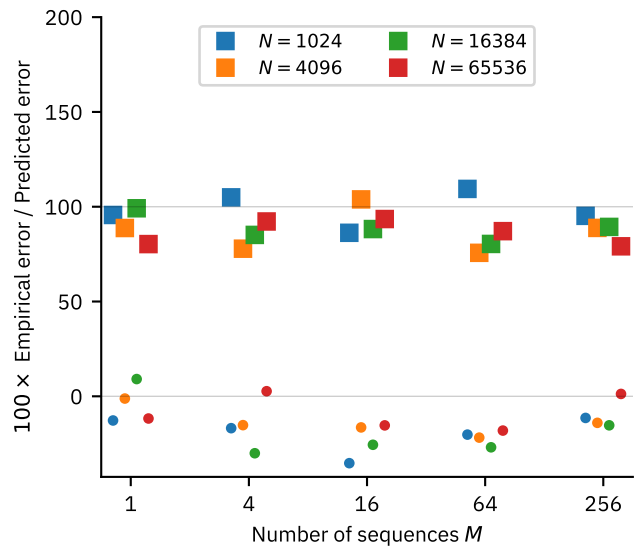
(a) Illustration of input data



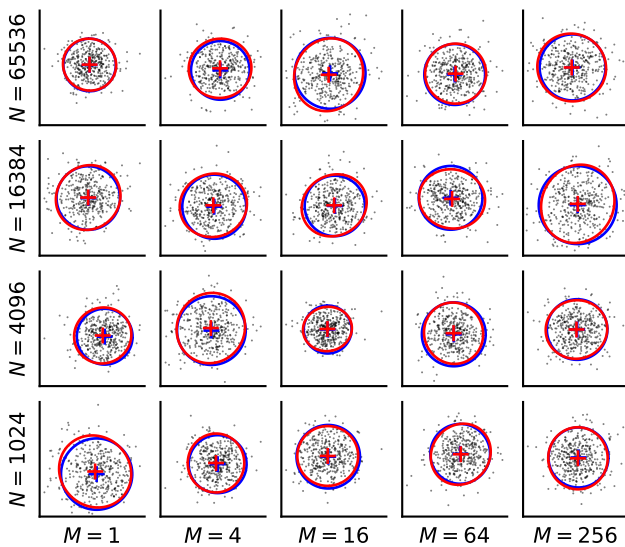
(b) Scaling of uncertainty of the autocorrelation integral with input data



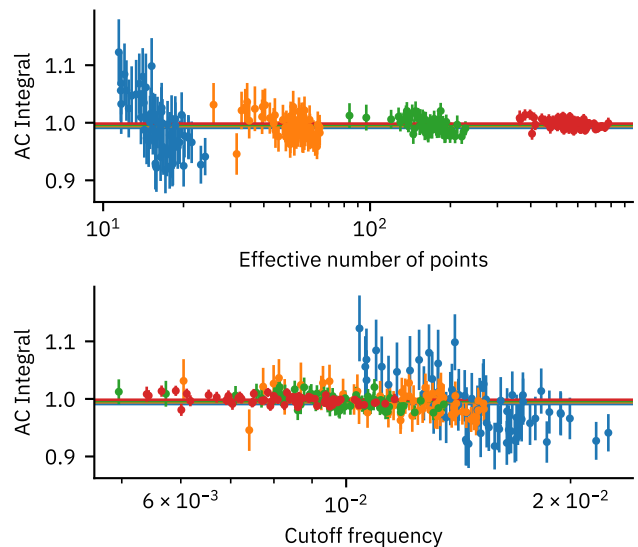
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	50	64	64	64	64
$N = 4096$	0	0	2	9	24
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

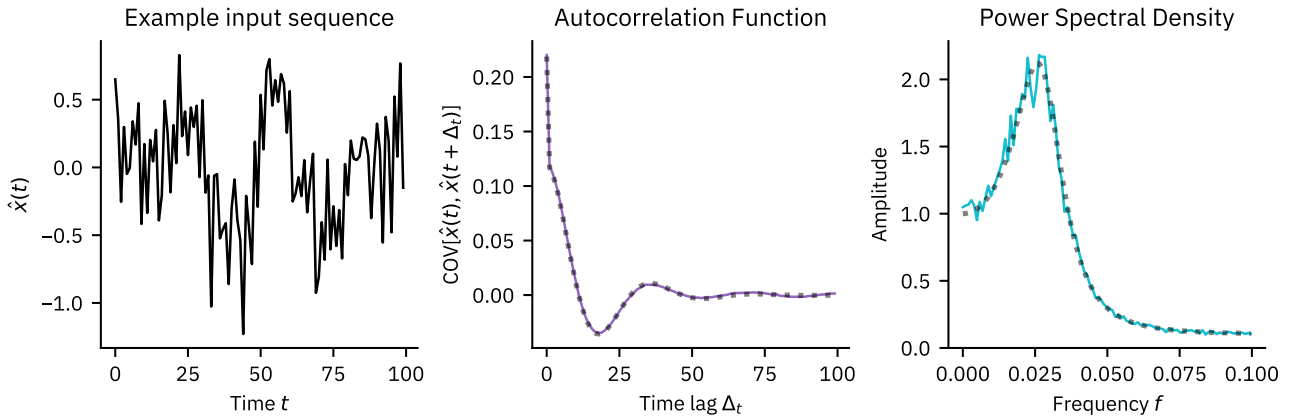
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	1	2	1	1
$N = 4096$	0	0	0	2	0
$N = 16384$	0	1	1	0	3
$N = 65536$	0	1	1	1	1

(i) Sanity check counts for the cutoff criterion z-score

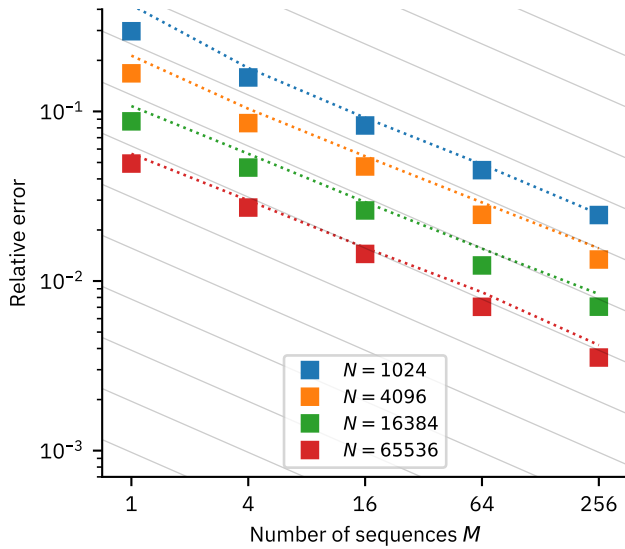
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	4	1	4	2	5
$N = 4096$	0	1	1	0	1
$N = 16384$	0	0	0	0	2
$N = 65536$	1	0	1	0	0

10. Kernel sho1wunder

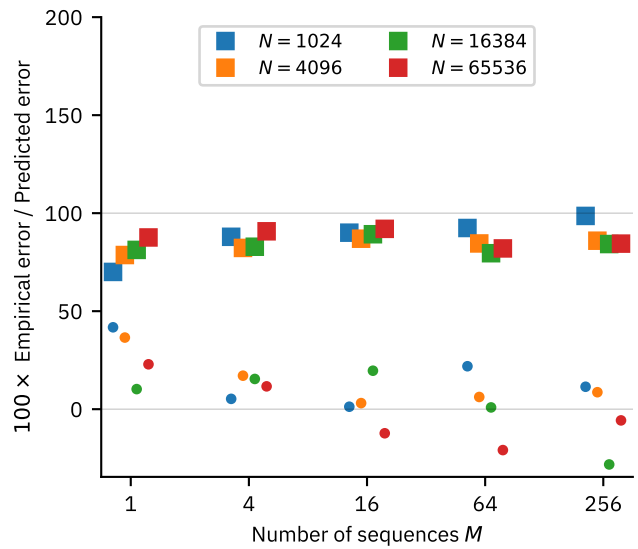
(a) Illustration of input data



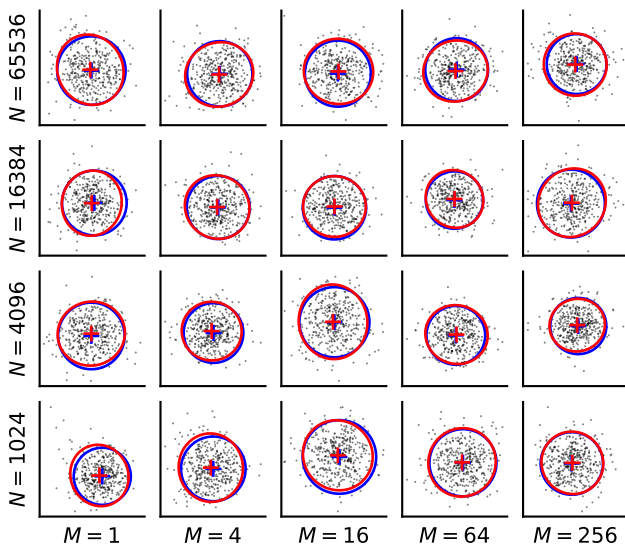
(b) Scaling of uncertainty of the autocorrelation integral with input data



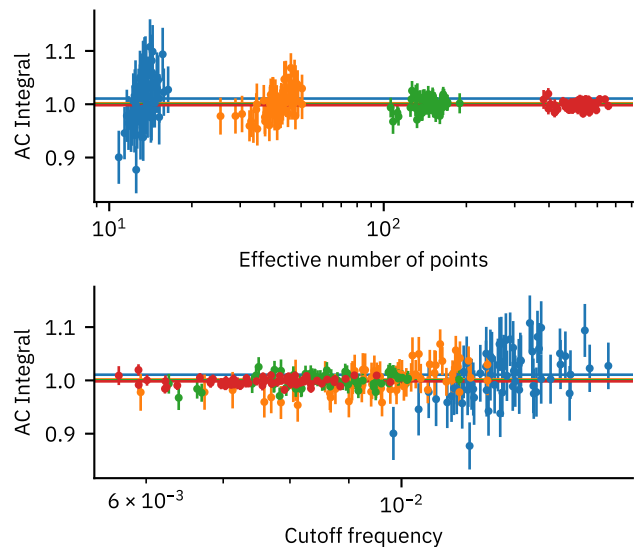
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	1	0	7	23	45
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

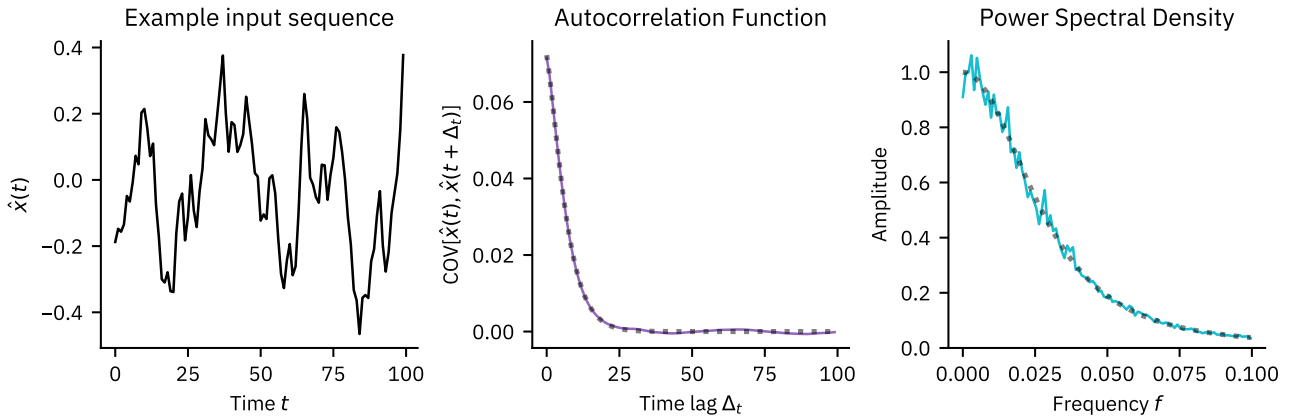
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	0	1	2	0
$N = 4096$	0	0	1	1	1
$N = 16384$	0	0	0	4	1
$N = 65536$	0	0	1	3	4

(i) Sanity check counts for the cutoff criterion z-score

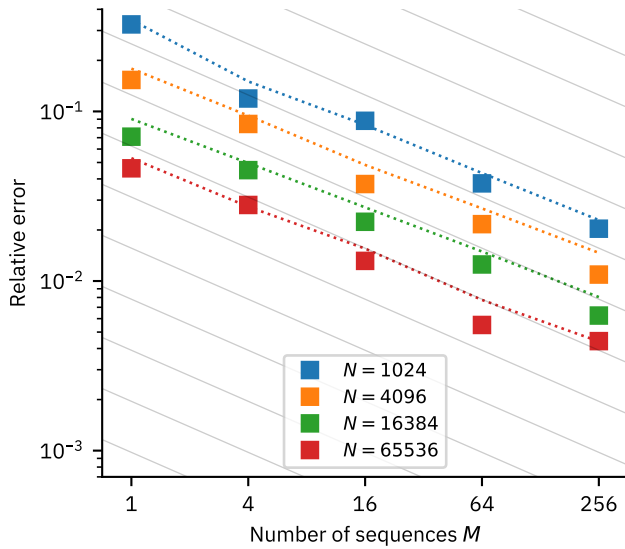
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	2	2	3	3	7
$N = 4096$	2	0	0	0	1
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	1	0

11. Kernel sho2crit

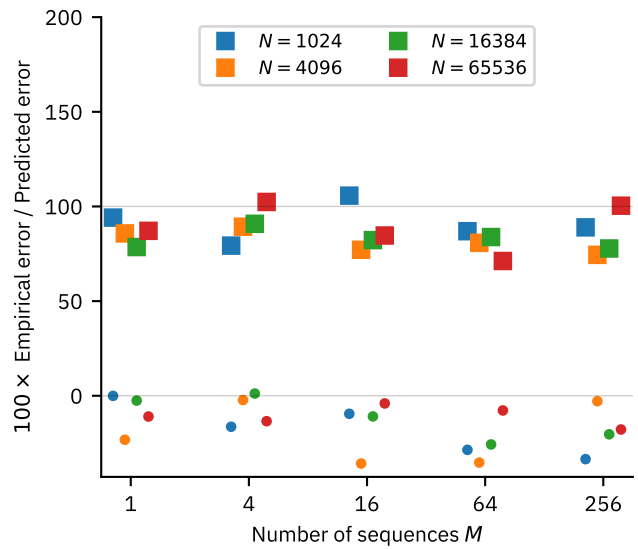
(a) Illustration of input data



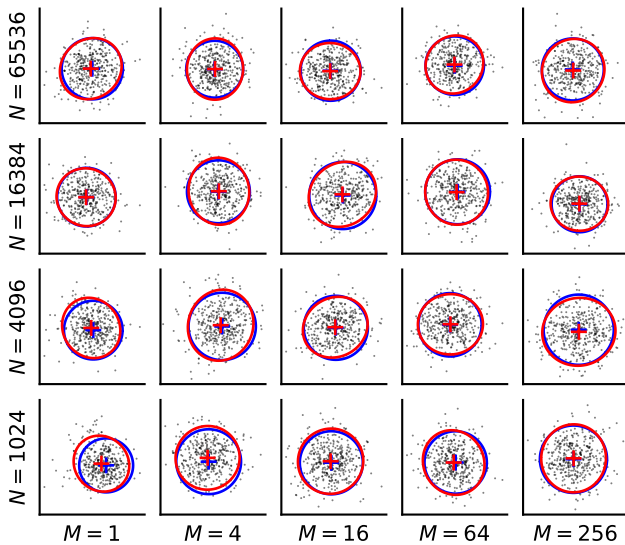
(b) Scaling of uncertainty of the autocorrelation integral with input data



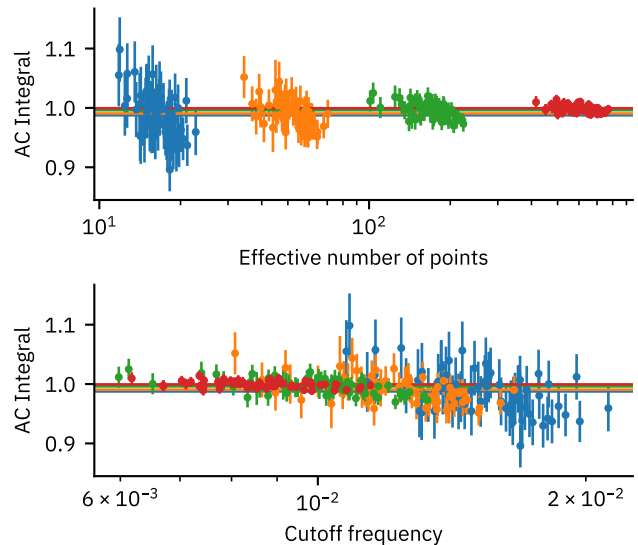
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	62	64	64	64	64
$N = 4096$	0	1	1	6	18
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

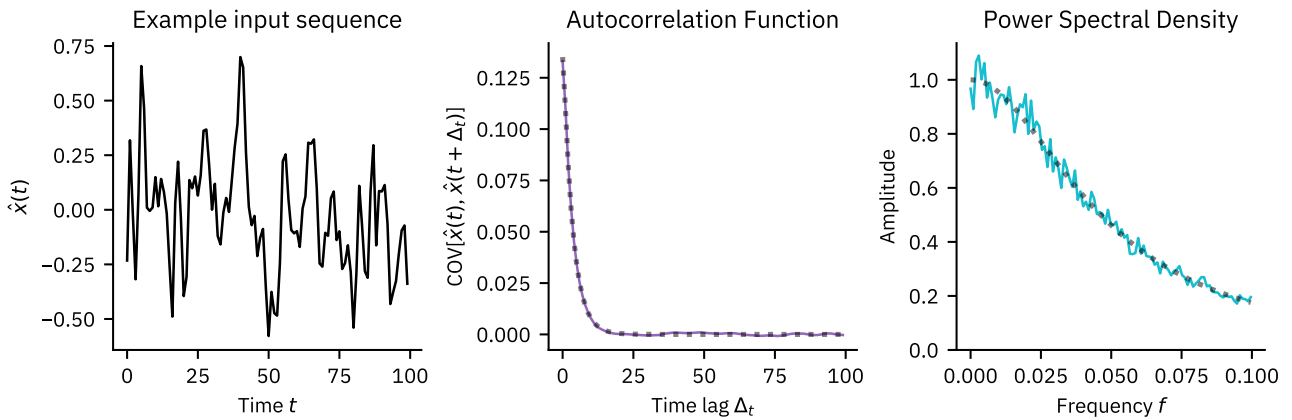
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	2	1	1	1
$N = 4096$	0	1	2	2	0
$N = 16384$	0	0	2	3	1
$N = 65536$	0	0	0	0	1

(i) Sanity check counts for the cutoff criterion z-score

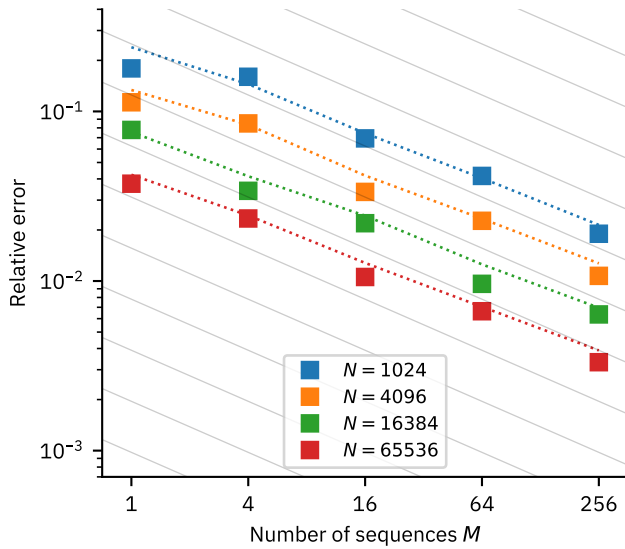
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	1	2	3	2	3
$N = 4096$	1	0	1	1	1
$N = 16384$	0	0	1	2	0
$N = 65536$	0	0	1	0	0

12. Kernel sho2over

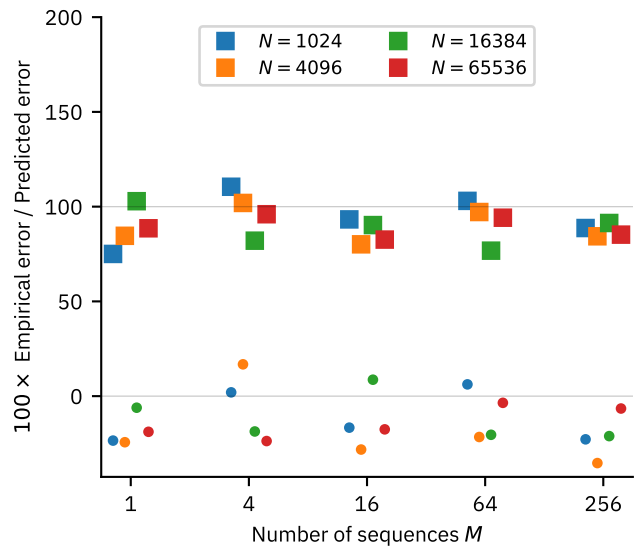
(a) Illustration of input data



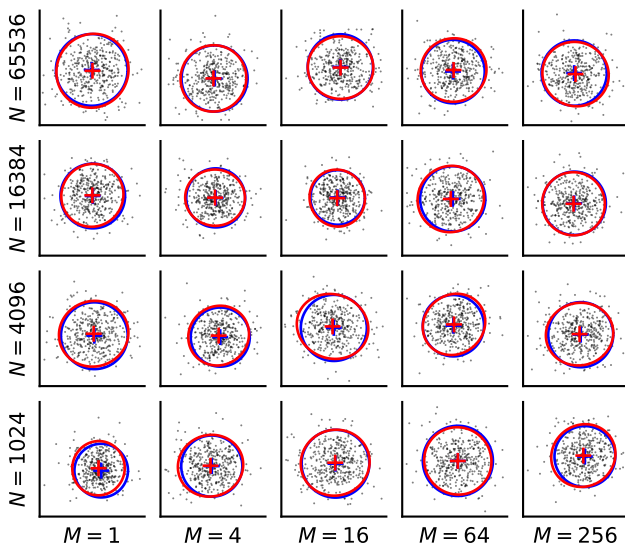
(b) Scaling of uncertainty of the autocorrelation integral with input data



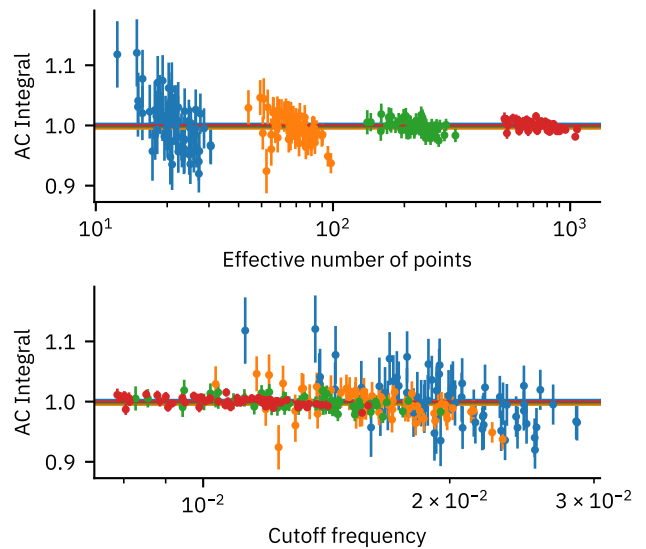
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	29	55	64	64	64
$N = 4096$	0	0	0	0	7
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

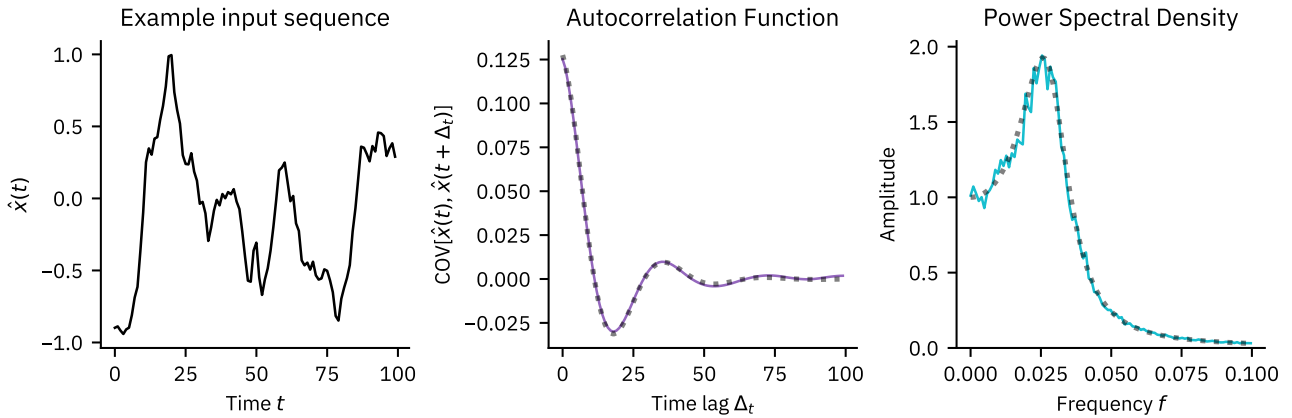
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	2	2	0	3
$N = 4096$	0	0	0	0	1
$N = 16384$	0	1	1	2	0
$N = 65536$	0	1	0	1	0

(i) Sanity check counts for the cutoff criterion z-score

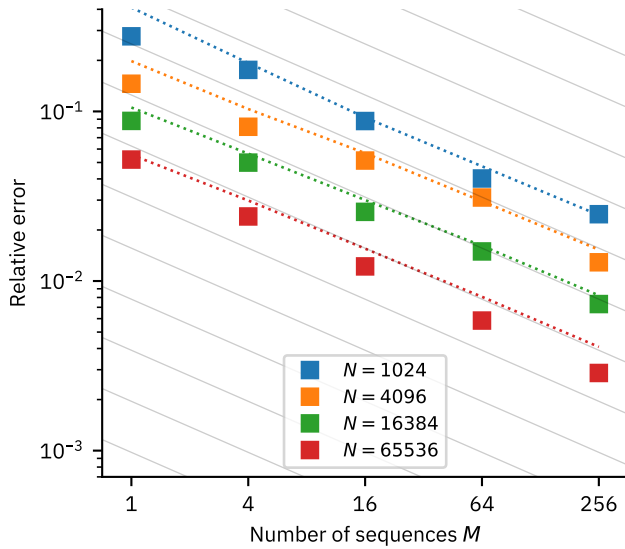
	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	1	3	3	2
$N = 4096$	1	3	0	0	0
$N = 16384$	0	0	1	0	0
$N = 65536$	0	1	0	0	0

13. Kernel sho2under

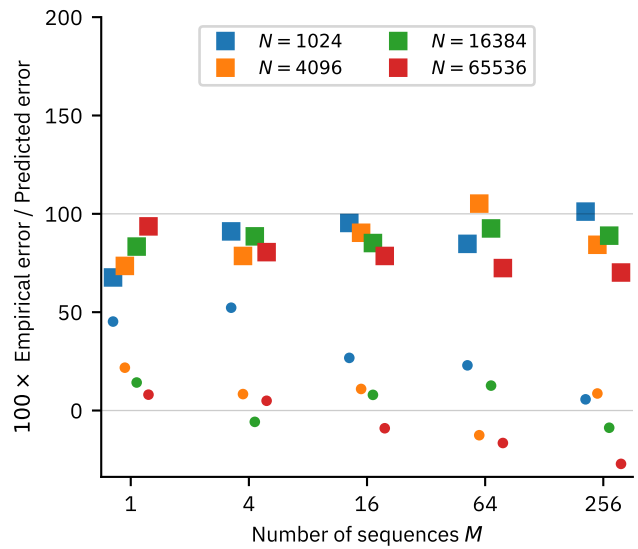
(a) Illustration of input data



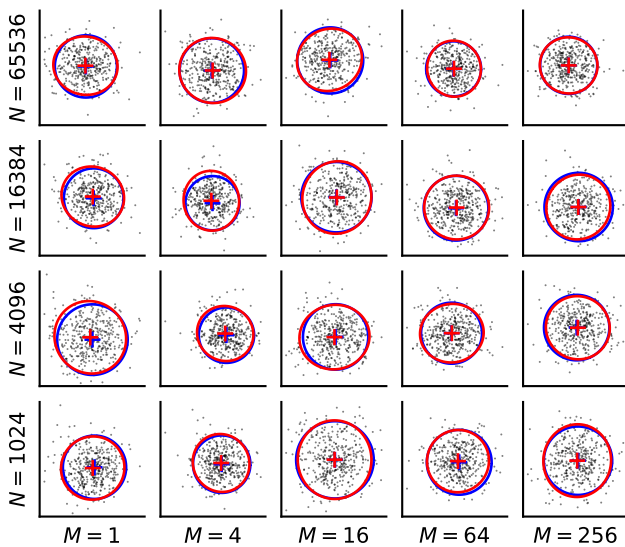
(b) Scaling of uncertainty of the autocorrelation integral with input data



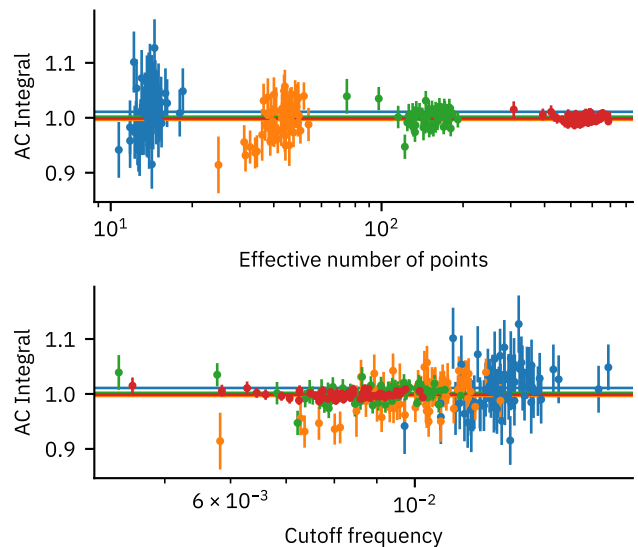
(c) Assessment of the error estimate of the autocorrelation integral



(d) Validation of the Maximum A Posteriori (MAP) estimate



(e) Sensitivity of the autocorrelation integral to the cutoff frequency



(f) Number of successful test cases

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	64	64	64	64	64
$N = 16384$	64	64	64	64	64
$N = 65536$	64	64	64	64	64

(g) Sanity check counts for the effective number of points

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	64	64	64	64	64
$N = 4096$	0	3	5	17	37
$N = 16384$	0	0	0	0	0
$N = 65536$	0	0	0	0	0

(h) Sanity check counts for the regression cost z-score

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	0	1	3	3	4
$N = 4096$	0	0	2	3	1
$N = 16384$	0	0	1	1	0
$N = 65536$	0	0	1	0	0

(i) Sanity check counts for the cutoff criterion z-score

	$M = 1$	$M = 4$	$M = 16$	$M = 64$	$M = 256$
$N = 1024$	1	1	5	3	10
$N = 4096$	0	0	1	0	0
$N = 16384$	0	0	1	0	0
$N = 65536$	1	1	0	0	0

Bibliography

- [1] G. Toraman, D. Fauconnier, and T. Verstraelen, “STable AutoCorrelation Integral Estimator (STACIE): Robust and accurate transport properties from molecular dynamics simulations,” *Journal of Chemical Information and Modeling*, vol. 65, no. 19, pp. 10445–10464, Sep. 2025, doi: [10.1021/acs.jcim.5c01475](https://doi.org/10.1021/acs.jcim.5c01475).